Indian J. Phys. **79(4)**, 367-371 (2005)

AN INTERNATIONAL JOURNAL
IJP

Thermal properties of copper and aluminum at high temperatures

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Received 22 June 2004, accepted 11 February 2005

Abstract : We investigate the thermo-elastic properties such as thermal expansion and expansivity of close packed phases of copper and aluminum upto their melting temperatures. The properties are calculated using the integral form of the equation of state (IFEOS) recently proposed by Singh and Gupta assuming the fact that the Anderson parameter (δ_T) strongly depends on temperature due to contribution from the thermal excitation of electrons. The values of thermal expansion (V/V_0), thermal expansivity (α_T) and bulk modulus (K_T) as determined in the present study, agree closely with the data based on temperature-dependent experimental studies.

Keywords : Thermal expansivity, bulk modulus, Cu, Al metals

PACS Nos. : 64.10.+h, 64.30.+t

1. Introduction

In the past few years, a number of scientists [1–3] have pursued the various methods to calculate the equation of state (EOS) of metals at high pressures and high temperatures. By using these equations of state, they have determined the pressure and specific internal energy of the metals as a function of density and temperature. The EOS provides a severe test to solid-state theories, as this depends on the nature of the interionic interactions present in the system. The thermal expansion, which is the function of interionic interaction, thus plays a central role in describing the high temperature behaviour of solids [4,5]. For practical purposes, the EOS provides an easy way to calculate and to predict a variety of thermo-elastic and thermodynamic properties of a given solid.

Among the number of isothermal and isobaric EOS described earlier [1–3, 6–8], we prefer the EOS due to Singh and Gupta [9] because of its simple and straightforward applications in high temperature physics. In the past, several equations of state have been derived within the Mie-Gruneisen approximation in terms of the low pressure, and the temperature-dependence is introduced into the EOS through some thermal pressure [10,11]. Vinet *et al* [12] then developed the temperature-dependent EOS by modelling the variations of bulk modulus with temperature and a known experimental value of the thermal expansion. This model is however, applicable under the assumption that the Anderson parameter (δ_T) is a temperature-independent and remains constant even in high temperature range. It has been recently noted [13] that the results on the temperature-dependent elastic properties improve if the linear dependence of Anderson parameter (δ_T) with temperature is assumed. This assumption has also been followed by Singh and Gupta [9] in obtaining the integral form of the EOS. In the present investigation, we have thus employed Singh and Gupta's (IFEOS) to calculate the thermal expansion and bulk modulus properties of metals Al and Cu. The aim of the present work is to extend our previous work further to test the validity and applicability of our previous EOS [9] to the variety of solids including metals. In Section 2, we have presented the method of analysis. The results obtained for Cu and Al metals, have been discussed in Section 3.

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2. Method of analysis

The standard definition of thermal expansivity (α_T) can be written as follows :

$$\alpha = \frac{1}{V}\left(\frac{dV}{dT}\right)_P . \tag{1}$$

The expression for the temperature dependence of α as obtained by Anderson *et al* [14] can be expressed as

$$\alpha = \alpha_0[1-\alpha_0\delta_T(T-T_0)]^{-1}, \tag{2}$$

where δ_T is the Anderson–Gruneisen parameter and is assumed to be a temperature-independent parameter. It is defined as

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{dK_T}{dT}\right)_P . \tag{3}$$

In view of eqs. (1) and (3),δ_T can also be written in the following form

$$\delta_T = -\frac{V}{K_T}\left(\frac{dK_T}{dV}\right)_P \tag{4}$$

or

$$\frac{dK_T}{K_T} = -\delta_T\left(\frac{dV}{V}\right). \tag{5}$$

By integrating eq. (5) at constant pressure, assuming that δ_T remains constant, we get

$$\frac{K_T}{K_T^0} = \left(\frac{V}{V_0}\right)^{-\delta_T} \tag{6}$$

or

$$\frac{V}{V_0} = \left(\frac{K_T}{K_T^0}\right)^{-\frac{1}{\delta_T}} . \tag{7}$$

The eq. (3) can also be rewritten as

$$\left(\frac{dK_T}{dT}\right)_P = -\alpha K_T\delta_T \tag{8}$$

which on integration, gives

$$K_T = K_T^0[1-\alpha_0\delta_T(T-T_0)]. \tag{9}$$

On substituting the eq. (9) into the eq (7), one may obtain the following expression for V/V_0.

$$\frac{V}{V_0} = [1-\alpha_0\delta_T(T-T_0)]^{-\frac{1}{\delta_T}} . \tag{10}$$

The equations (2, 9 and 10) have been derived earlier [14] under the high temperature approximation, assuming that the Anderson parameter δ_T and the product αK_T are temperature-independent parameters. Motivated with this situation, Singh and Gupta [9] have recently derived the integral form of the equation of state (IFEOS) considering the fact that δ_T varies with temperature and hence, cannot be assumed temperature-independent parameter. However, the product αK_T is assumed to be constant and thus is a temperature-independent parameter in our formulation, too. Our assumption in the present investigation is quite consistent with the equilibrium condition of the crystal at the reference temperature T_0, the calculated values correspond to the room temperature values or the experimental values measured at room temperature. The empirical dependence of Anderson-Gruneisen parameter (δ_T) with temperature is assumed as [15,16]

$$\delta_T = \delta_T^0(X)^k , \tag{11}$$

where δ_T^0 is the value of Anderson-Gruneisen parameter at $T = T_0$, and $X = T/T_0$, T_0 is the reference temperature. k is the dimensionless thermo-elastic parameter which can be calculated from the slope of the graph plotted between log δ_T and log (T/T_0). On substitution of eq (11) into the eq. (3) and following the procedure of the previous workers [9], we obtained the following new expression for K_T/K_0,

$$\frac{K_T}{K_0} = \left[1-\frac{\alpha_0\delta_T^0}{T_0^k(k+1)}\left(T^{k+1}-T_0^{k+1}\right)\right]. \tag{12}$$

The expression for thermal expansion (V/V_0) can similarly be obtained by making use of eq. (5) as follows :

$$dK_T = -K_T\delta_T\frac{dV}{V} . \tag{13}$$

By differentiating the eq. (12), we can get,

$$dK_T = -\frac{\alpha_0 K_0\delta_T^0}{T_0^k}T^k dT . \tag{14}$$

Substituting eq. (14) into the eq. (13), we get

$$\frac{dV}{V} = \frac{\alpha_0}{\left[1-\frac{\alpha_0\delta_T^0}{T_0^k(k+1)}(T^{k+1}-T_0^{k+1})\right]}dT . \tag{15}$$

The integration of eq. (15) gives us the new equation of state for thermal expansion, which is finally defined as

$$\frac{V}{V_0} = \exp\left[\int_{T_0}^{T} \frac{\alpha_0}{\left[1 - A\left(T^{k+1} - T_0^{k+1}\right)\right]} dT\right], \quad (16)$$

where $A = \alpha_0 \delta_T^0 / T_0^k (k+1)$. Similarly, the expression for thermal expansivity obtained by Singh and Gupta [9] can be written as

$$\frac{\alpha_T}{\alpha_0} = 1 - \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)} \left(T^{k+1} - T_0^{k+1}\right)^{-1} \quad (17)$$

The expressions (12, 16, 17) have already been used by Singh and Gupta to explain the thermo-elastic properties of minerals CaO and MgO. An excellent agreement with the available experimental data has been reported.

In the present investigation, we have used these equations for the time to predict the thermal expansion and bulk modulus properties of metals (Cu and Al) under the effect of high temperature. Though the various approaches based on potential model have been used earlier, yet our method of calculation is not only simple and straightforward but also predicts better results as compared to those obtained by using potential models.

3. Results and discussion

Our present results confirm that the integral form of EOS determines the temperature-dependence of the thermo-dynamical properties of metals as good as of the minerals. The values of input data used in the present EOS are given in Table 1.

Table 1. Input data taken from Refs. [17,21].

Metals	α_0 ($10^{-5}K^{-1}$)	K_0 (GPa)	δ_T^0
Cu	5.04	133	5 7
Al	6.96	72.8	7.76

It can be noted from the Tables 2 and 3 that the values of thermal expansion, thermal expansivity and bulk modulus as achieved in the present work for Cu and Al metals, are very close to the available experimental values. The calculated values are plotted with temperature and compared with experimental values and also with those calculated by previous workers [17–20,22]. It is evident from the graphs that the results obtained by using the eqs. (12, 16, 17), are much better than those values predicted by using the various potential models [22]. The value of thermo-elastic parameter (k) in this equation has been found as −0.017 for copper (Cu) and −0.23 for aluminum (Al).

Table 2. Values of V/V_0, α_T (in unit of $10^{-5}K^{-1}$) and K_T (GPa) for Cu.

Temperature (K)	Calculated in present study			Experimental from [17–20]			Values taken [22]	
	V/V_0	α_T	K_T	V/V_0	α_T	K_T	V/V_0	α_T
300	1	5.04	133	1	5.04	133	–	–
400	1.0051	5.18	129.2	1 0052	5.18	129.5	1.0055	5.28
500	1.0104	5.35	125.3	1.011	5.35	124.5	1.0109	5.49
600	1.0159	5 51	121.5	1.0164	5.53	121.8	1.0166	5.67
700	1.0216	5.69	117.8	1.0215	5.71	118.2	1.0224	5.85
800	1.0276	5.87	114.1	1.0287	5.89	115	1.0284	6.09
900	1.0337	6.08	110.2	1.0338	6.12	–	1.0348	6.39
1000	1.0401	6.29	106.5	1.0403	6.33	–	1.0415	6.72
1100	1.0468	6.53	102.7	1.0472	6.53	–	–	–
1200	1.0538	6.77	99	1.0551	6.82	–	1.0562	7.47
1300	1.0611	7.03	95.3	1.0626	7.32	–	1.0642	7.74

Table 3. Values of V/V_0, α_T (in unit of $10^{-5}K^{-1}$) and K_T (GPa) for Al.

Temperature (K)	Calculated in present study			Experimental from [17–20]		Values taken [22]	
	V/V_0	α_T	K_T	α_T	K_T	V/V_0	α_T
300	1	6.96	72.8	6 96	72.8	1	–
350	1.0035	7.15	70.9	7.23	71.3	–	–
400	1 0072	7.34	69.0	7.47	69.6	1.008	7.53
450	1.0109	7.54	67.2	7.68	67.8	–	–
500	1.0148	7 75	65.4	7.92	65.8	1.0156	7.92
550	1.0188	7.97	63 6	8.18	63.5	–	–
600	1.0229	8.19	61.9	8.49	61.0	1.0238	8.52
650	1.0272	8.40	60.3	–	–	–	–
700	1.0315	8.63	58.7	–	–	1 0329	9.27
750	1.0361	8.87	57.1	–	–	–	–
800	1.0407	9.13	55.5	–	–	1.0428	10.20

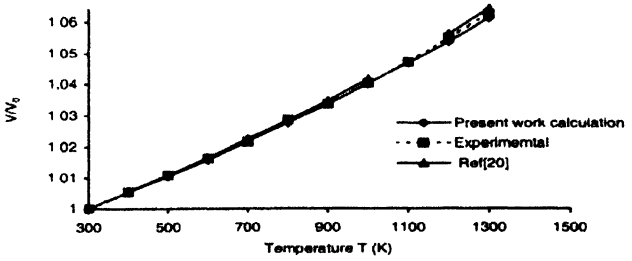

Figure 1. Variation of relative thermal expansion (V/V_0) with temperature for Cu.

On the basis of overall discussions, it may be concluded that our model merits the attention for the selection of the reference thermodynamic state required to generate the EOS, since one may select any class of solids. Our methodology is useful especially for solids (variety structure solids), which have the Debye temperature Θ_D value higher than the room temperature.

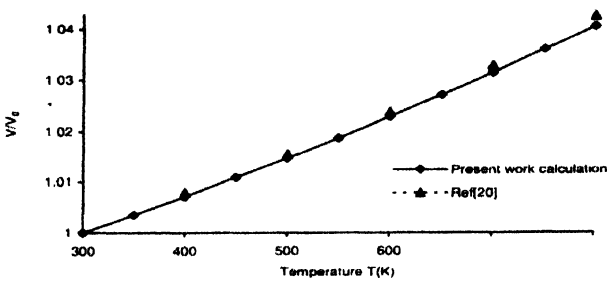

Figure 2. Variation of relative thermal expansion (V/V_0) with temperature for Al.

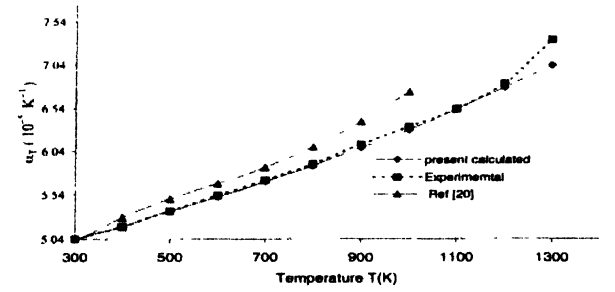

Figure 3. Variation of thermal expansivity (α_T) with temperature for Cu.

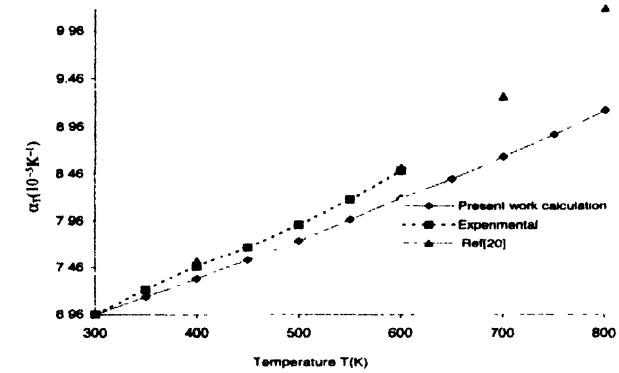

Figure 4. Variation of thermal expansivity (α_T) with temperature for Al.

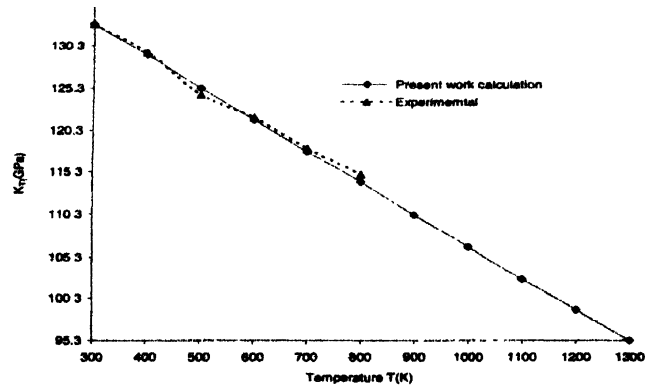

Figure 5. Variation of bulk modulus (K_T) with temperature for Cu.

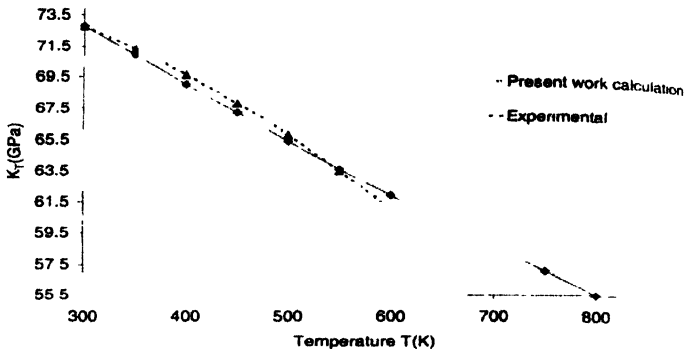

Figure 6. Variation of bulk modulus (K_T) with temperature for Al.

This study may have tremendous impact in high-pressure or high-temperature researches where the results at different temperatures are required.

Acknowledgment

The authors are thankful to the referee for his valuable comments and suggestions. The present research work supported by the Council of Scientific and Industrial Research (New Delhi, India), under research Project No. 03 (0939)/02/EMR-II, is duly acknowledged.

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